2,3,4,9-tetrachlorodibenzofuran

Other names: Dibenzofuran, 2,3,4,9-tetrachloro
1,6,7,8-Tetrachlorodibenzofuran
Inchi: InChI=1S/C12H4Cl4O/c13-6-2-1-3-8-9(6)5-4-7(14)10(15)11(16)12(5)17-8/h1-4H
InchiKey: KOJMOXYETDLOPN-UHFFFAOYSA-N
Formula: C12H4Cl4O
SMILES: Clc1cc2c(oc3cccc(Cl)c32)c(Cl)c1Cl
Mol. weight [g/mol]: 305.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.55		Crippen Method
logp	6.200		Crippen Method
mcvol	176.390	ml/mol	McGowan Method
rinpol	2308.00		NIST Webbook
rinpol	2318.00		NIST Webbook
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
rinpol	2318.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R29784&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices